

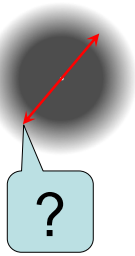


Relationship between mobility and diameter of singly charged spherical symmetric aerosol particles

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Workshop presentation 20120201






Introduction:



- concept of diameter,
- mobility and mobility model,
- basic theoretical models,
- who made the Millikan model?
- ISO15900,
- updating the Millikan model,
- why the new models do'n't have success?

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A selection of diameters



The aerodynamic diameter is defined as the diameter of a spherical particle of unit density having the same terminal settling velocity as that of the particle in question. The aerodynamic diameter is useful for particles having appreciable inertia, that is, those larger than about 0.5 μm. Particles smaller than about 0.5 μm undergo Brownian motion and are characterized by the diffusive diameter, the diameter of a particle that has the same diffusion coefficient as the particle in question. The electrical mobility diameter is the diameter of a spherical particle with the same electrical mobility as that of particle in question. The Stokes diameter is the diameter of a spherical particle having the same density and settling velocity as the particle in question. An optical diameter is defined as the diameter of a particle having the same response in an instrument that detects particles by their interaction with light. There are a number of diameter definitions

.....volume diameter (Larriba et al. 2011, AST 45, 453-467)

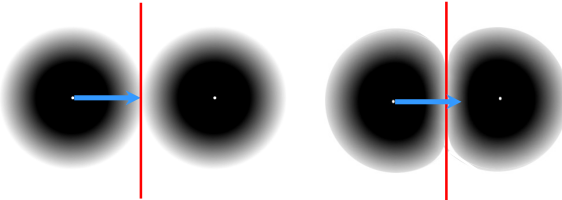
All these definitions expect that the diameter of a spherical particle is a well defined quantity.

from: Kulkarni, Baron Willeke
Aerosol measurement

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Nanoparticles have “atmospheres”, no solid surface



Density functions of two colliding nanoparticles

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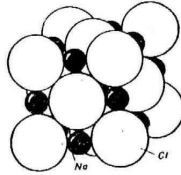





A similar problem:

Atomic radii are required when assembling the crystal models.

The radius of the same atom is a variable depending on the bonds. E.g. Na in the metallic sodium is much bigger than in a NaCl crystal.





Slater (1964) proposed a specific mean radius as a universal parameter:

Atom	H	O	N	Na	Cs
2×R _s : nm	0.05	0.12	0.13	0.36	0.52

The Slater radius of an orbital is the distance where the density of probability to find the electron has maximum. However the mean square deviation of real distances in crystals from the Slater distances is still about 0.012 nm.

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Mass diameter $d = \sqrt[3]{\frac{6m}{\pi\rho}}$

NB: $\rho \neq$ density of bulk matter
 ρ = density of particle matter

An array of packed spheres has the density of
0.52 ρ in case of the simple cubic lattice and
0.74 ρ in case of the closest packing.

Mason, E.A. (1984) Ion mobility: its role in plasma chromatography. In Plasma Chromatography (Edited by T.W. Carr), 43–93. Plenum Press, New York and London.

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Mobility and mobility model

Precondition: the mean drift velocity v is proportional to the drag force F .



Mechanical mobility $B = v/F$, electrical mobility $Z = v/E$
 $F = Eq$ follows in $Z = qB$. We have $q = e$ and $Z = eB$.

A model of mobility is an algorithm that uses parameters of the particle and the air (pressure, temperature, diameter etc.) and issues an estimate of the particle mobility:

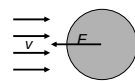
$Z \approx Z_M = f_M(p, T, d)$ or $Z \approx Z_M = f_M(p, T, \dots, d)$.

The inverse model $d \approx d_M = g_M(p, T, Z)$ is to be mathematically derived from the direct algorithm.

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Theoretical basic models



The **Newton model** of drag is nonlinear

$$F = c_x \frac{\rho_g v^2}{2} \frac{\pi d^2}{4} \approx 0.2 \rho_g d^2 v^2$$

cross section

Speed and fictive mechanical mobility

$$v \approx \frac{\sqrt{5F/\rho_g}}{d} \quad B \approx \frac{\sqrt{5/(F \times \rho_g)}}{d}$$

Stokes model of drag is linear



$$F = 3\pi\eta dv \quad B = \frac{1}{3\pi\eta d} \quad Z = \frac{e}{3\pi\eta d}$$

Rigid sphere model by Chapman ja Enskog
in first approximation $\Omega = \Omega^{(1,1)}$ and $\Omega^{(1,1)} = \pi r^2$

$$B = \frac{3}{2(d_g + d_p)^2 n_g} \sqrt{\frac{(1 + m_g/m_p)}{2\pi m_g kT}} \bigg/ s$$

Epstein (1924) calculated effect of diffuse impacts on drag of about $s = 1.32$

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Mobility diameter

Mobility diameter is defined as the diameter of a hard sphere of the same mobility as the considered particle. Thus the mobility diameter of a spherical particle is just the same as its geometric diameter.

Sometimes the mobility diameter is considered as a value d_M issued by a specific mobility model

$d_M = g_M(p, T, Z)$,

where g_M is inverse function of the model M and Z is measured mobility. The choice of the specific model is free, one could choose even plain Stokes or Newton. Thus d_M should not be considered as a physical quantity. It is a specific estimate of the diameter.

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Wang, H. (2009) Transport properties of small spherical particles. Ann. N.Y. Acad. Sci. 1161, 484–493.

Transport Properties of Small Spherical Particles

Hai Wang

Aerospace and Mechanical Engineering Department, University of Southern California, Los Angeles, California, USA

Recently, a theoretical framework for nanoparticle transport in the laminar flow regime has been proposed. The theory features a rigorous gas-kinetic theory analysis. It considers the effect of nonrigid body collision, and the theory is shown to reproduce the Chapman-Enskog theory of molecular transport in the small particle size limit, Epstein's model of particle drag in the rigid-body limit, and the Stokes-Cunningham equation for the drag on micrometer size particles. This theoretical framework provides the hope that bits and pieces of particle transport theories formulated over the last century can now be unified into a generalized theory. This paper discusses an **unresolved fundamental issue** related to this generalized theory, namely, the transition from specular scattering applicable to molecule-molecule collision to diffuse scattering governing molecule-"particle" collision.

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Comparison of models



$B : (m/s) / fN$ is the speed (m/s) caused by force of $10^{-15} N$

$$B_{Stokes} = \frac{10^{-15}}{3\pi\eta d} \quad B_{Chapman(RS)} = \frac{5.98 \times 10^{-16}}{(d_g + d_p)^2 n_g} \sqrt{\frac{1/m_g + 1/m_p}{kT}}$$

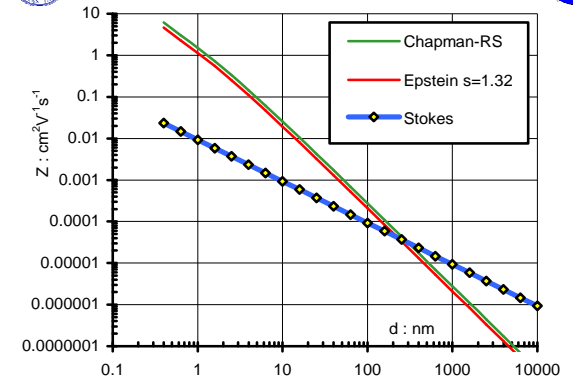
$$Z : cm^2 / (Vs) = 1.6022 \times B : (m/s) / fN$$

Values of parameters (gaas = õhk, mõõtühikud SI):

$$\begin{aligned} \rho &= 101325 \text{ Pa}, \quad T = 273.15 \text{ K}, \quad \rho_p = 2000, \\ \rho_g &= 1.293, \quad k = 1.38E-23, \quad \eta = 1.736E-5, \\ d_g &= 3.74E-10, \quad n_g = 2.687E+25, \quad m_g = 4.809E-26, \end{aligned}$$



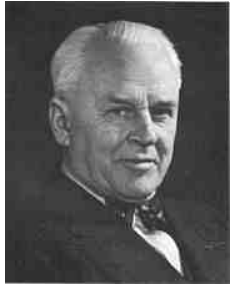
Comparison of mobility models



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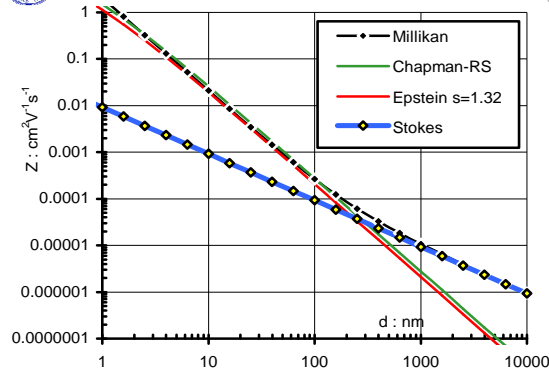


There is no likelihood man can ever tap the power of the atom. The glib supposition of **utilizing atomic energy** when our coal has run out **is a completely unscientific Utopian dream, a childish bug-a-boo**. Nature has introduced a few fool-proof devices into the great majority of elements that constitute the bulk of the world, and they have no energy to give up in the process of disintegration.

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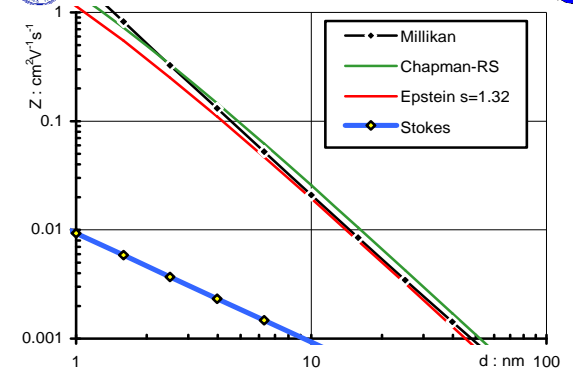
Comparison of mobility models



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Comparison of mobility models



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Who made the Millikan model?



Ebenezer Cunningham



Martin Knudsen
(no Jens)



Moritz Weber



Robert Andrews Millikan

THE PHYSICAL REVIEW
LANCASTER, PA., AND ITHACA, N. Y.
1913

ON THE ELEMENTARY ELECTRICAL CHARGE AND THE
AVOGADRO CONSTANT.

By R. A. MILLIKAN.

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Millikan model



$$Z = \left(1 + Kn \left(A + B \exp \left(-\frac{C}{Kn} \right) \right) \right) \frac{q}{3\pi\eta d} \quad Kn = \frac{l}{r} = \frac{2l}{d}$$

Millikan 1923:	A = 0.864	B = 0.29	C = 1.25
Davies 1945:	A = 1.257	B = 0.400	C = 0.55
Allen & Raabe 1985:	A = 1.142	B = 0.558	C = 0.999
Tammet 1995:	A = 1.2	B = 0.5	C = 1
Kim et al. 2005:	A = 1.165	B = 0.483	C = 0.997
Jung et al. 2011:	A = 1.165	B = 0.480	C = 1.001

Kim, J.H., Mulholland, G.W., Kukuck, S.R., Pui, D.Y.H. (2005)
Slip correction measurements of certified PSL nanoparticles using a nanometer differential mobility analyzer (Nano-DMA) for Knudsen number from 0.5 to 83. J. Res. Natl. Inst. Stand. Technol. 110, 31–54.

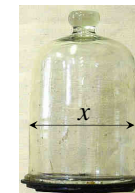
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Knudsen



Martin Hans Christian Knudsen (1871 - 1949) was a Danish physicist at the Technical University of Denmark. He is primarily known for his study of molecular gas flow and the development of the Knudsen cell, which is a primary component of molecular beam epitaxy systems. His book, The Kinetic Theory of Gases (London, 1934), contains the main results of his research.



From basic physics:
what is the measure of the vacuum?

$$l - \text{free path} \quad x - \text{flight range} \quad Kn = \frac{l}{x}$$

NB: nanometer particles in atmospheric air are surrounded by vacuum.

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(Pseudo)problem of free path

See Jennings (1988)

$$Z = \left(1 + Kn \left(A + B \exp\left(-\frac{C}{Kn}\right)\right)\right) \frac{q}{3\pi\eta d} \quad Kn = \frac{l}{r} = \frac{2l}{d}$$

In old books $l = 3D/\nu \approx 90$ nm, in new books $l \approx 2D/\nu \approx 60$ nm

$$Z = \left(1 + \frac{2}{d} \left(Al + Bl \exp\left(-\frac{d}{2} \times \frac{C}{l}\right)\right)\right) \frac{q}{3\pi\eta d}$$

Now the free path is everywhere in combination with one of the coefficients A, B, C and effect of changed value of l can be exactly compensated with a change in values of A, B, C.

Jung et al. 2011: $A = 1.165$ $B = 0.480$ $C = 1.001$
 Updated Millikan: $A = 1.296$ $B = 0.435$ $C = 0.833$
 Millikan 1923: $A = 0.864$ $B = 0.29$ $C = 1.25$

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ISO15900

Recommended values for S_c , η and l

The electrical mobility Z of a particle depends on its size d and its electric charge p . The relationship between electrical mobility and particle size for spherical particles is a function of the slip correction S_c , the dynamic viscosity η and the mean free path l of gas molecules according to the following equations:

$$Z(d, p) = \frac{pC}{3\pi\eta d} S_c \quad S_c = 1 + Kn \left[A + B \exp\left(-\frac{C}{Kn}\right)\right] \quad Kn = \frac{2l}{d}$$

$$l = l_0 \times \left(\frac{T}{T_0}\right)^2 \times \left(\frac{P_0}{P}\right) \times \left(\frac{T_0 + S}{T + S}\right) \quad \text{Sutherland, 1893} \rightarrow \eta = \eta_0 \times \left(\frac{T}{T_0}\right)^{3/2} \times \left(\frac{T_0 + S}{T + S}\right)$$

Parameter	Value	Remarks
η_0	$1.832 \cdot 45 \cdot 10^{-5} \text{ kg m}^{-1} \text{ s}^{-1}$	
l_0	$6.730 \times 10^{-8} \text{ m}$	For dry air at $T_0 = 296.15 \text{ K}$; $P_0 = 101.3 \text{ kPa}$.
S	110.4 K	All values from:
A	1.165	J.H. Kim, G.W. Mulholland, S.R. Kukucki and D.Y.H. Pui (2005).
B	0.483	
C	0.997	

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Updating the Millikan model

Original model $Z = Z_{\text{Millikan}}(p, T, d)$ does not consider:

- polarization interaction between ions and gas molecules,
- size and mass of gas molecules,
- transition from diffuse scattering of molecules to the elastic-specular collisions.

First update: the diameter complement

$$Z = Z_{\text{Millikan}}(p, T, d + \Delta d)$$

Standard collision diameter of "air molecules" = **0.37 nm**

Tammet (1995) (at $d \rightarrow \text{infinity}$): $\Delta d \rightarrow$ **0.6 nm**

Fernandez de la Mora et al. (2003): $\Delta d =$ **0.53 nm**

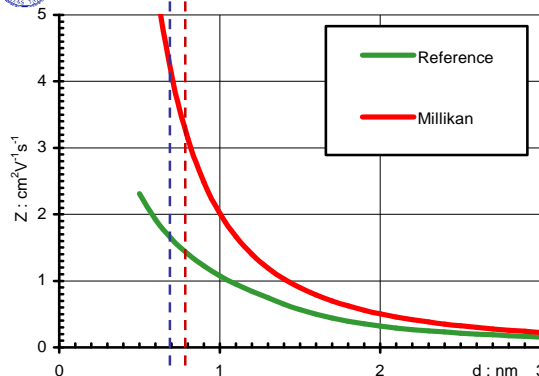
Ku et al. (2009): $\Delta d =$ **0.3 nm**

Larriba et al. (2011): $\Delta d =$ **0.3 nm**

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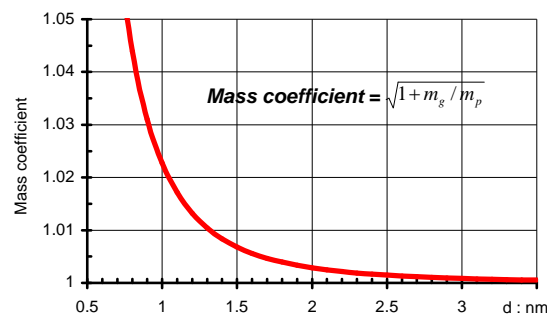
Comparison of mobility models



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Second update: $Z = Z_{\text{Millikan}} \cdot \text{Mass coefficient}$



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A selection of newer models

Tammet, H. (1995) Size and mobility of nanometer particles, clusters and ions. J. Aerosol Sci. 26, 459–475.

Li, Z., Wang, H. (2003) Drag force, diffusion coefficient, and electric mobility of small particles. II. Application. Phys. Rev. E 68, 061207.

Shandakov, S.D., Nasibulin, A.G., Kauppinen, E.I. (2005) Phenomenological description of mobility of nm- and sub-nm-sized charged aerosol particles in electric field. J. Aerosol Sci. 36, 1125–1143.

Wang, H. (2009) Transport properties of small spherical particles. Ann. N.Y. Acad. Sci. 1161, 484–493.

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Bibliometry

Citations in 2010 ja 2011 recorded in WebOfScience (paper by Ku et al. was published 2009):

Li and Wang (2003)	8
Ku et al. (2009)	20
Tammet (1995)	26

Google search:	all years	2007-2011
"Millikan diameter"	43	14
"Tammet diameter"	32	6

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Poor success of new models

The model by Li and Wang (2003) is based on the most developed theory. However, Google did not find any application of this model in aerosol measurements. The same can be told about the model by Shandakov et al. (2005). Few references are found only inside of block references in introductions of the papers.

Reasons?

1. No simple computing algorithm available.
2. No comprehensible interpretation available.

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Poor success of new models

The model by Tammet (1995) have had few applications. The detailed algorithm is available, but long and cumbersome. There is no simple interpretation. Mäkelä et al. (1996) made an attempt to find a simplified formal approximation:

$$Z_p = \frac{1}{10000} \left[-0.1831 \cdot D_p^8 + 2.3982 \cdot D_p^7 - 13.1331 \cdot D_p^6 + 38.8578 \cdot D_p^5 - 66.7785 \cdot D_p^4 + 65.9213 \cdot D_p^3 - 32.7985 \cdot D_p^2 + 2.7702 \cdot D_p + 4.0377 \right],$$

where D_p is given in nm's and Z_p in m^2/Vs .

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End of the introduction

Proposal and discussion of a new model



New approach

In sake of convenience and accustomed interpretation:

the new model is made up of the Millikan equation with a diameter complement.

With an aim to take into account the peculiarities of $d < 3$ nm particles:

the diameter complement is considered as a function of the particle mass diameter,

and when required, of the air temperature and pressure:

$$\Delta d = f(d) \quad \text{or} \quad \Delta d = f(p, T, d).$$

(so far Δd was considered as a constant)

Problem: how to determine this function and how to assure simplicity of applications?

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Determining of $\Delta d = f(d)$

At the first glance it seems to be a similarity with the Cunningham-Knudsen-Weber-Millikan task to find a good approximation for the slip factor.

However, there is a fundamental difference:

- ▶ slip factor depends on the Kn that can obtain high value in case of relatively large particles at low pressure,
- ▶ Δd depends immediately on the particle size and cannot be controlled by pressure.

Thus the low pressure experiments with large particles are not helpful and the experiments should be made with sub-3 nm spherical particles of exactly known size.

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Determining of $\Delta d = f(d)$

1. Get a reference table of precise measurements or an exact reference model of $Z = f(d)$. The reference model may have no requirements for simple interpretation and computation.
2. Choose parameters of air p , T and a diameter d_1 ,
3. Get the accurate mobility $Z = Z(d_1)$ from the reference table or compute it by means of the reference model.
4. Calculate by means of plain ISO15900 Millikan model ($\Delta d = 0$) a diameter d_2 that corresponds to Z obtained in p.3.
5. Calculate the diameter complement $\Delta d = d_2 - d_1$.

Now the result of plain Millikan equation at $d_1 + \Delta d$ is exactly the same as the reference mobility. We will get different value of Δd for every d in the range of $d < 3$ nm and should compile a representative table of function $\Delta d = f(d)$.

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Determining of $\Delta d = f(d)$

Next task is: to find a good approximation for the tabulated function $\Delta d = f(d)$.

The task is a bit similar to the Cunningham-Millikan problem of looking for approximation the slip correction factor. Unfortunately, we have no physical idea and the search for the approximation is considered as a formal procedure based on intuition and numerical methods of computational mathematics.

A remark: The reference table of measurements of the function $\Delta d = f(d)$ is strongly preferred. Such a table was not available when compiling the presentation and following examples are designed using a reference model.

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The reference model

The reference model was based on the $Z = f(d)$ model by Tammet (1995) because the lack of well prepared alternatives. The original model was modified because

the approximations of the air viscosity, free path and slip factor coefficients A, B, C should be the same in the Millikan equation and in the reference model. These approximations are prescribed in ISO15900.

Exception: Standard values $B = 0.483$, $C = 0.997$ may be replaced with recent results $B = 0.480$, $C = 1.001$.

These changes were entered into the algorithm and the result *Tammet95m* was used as a tentative reference model.

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The reference model

$$Z = f(p, T, p, q, d)$$

```
function electrical_mobility_air (Tammet95m)
  (Millibar, Celsius, ParticleDensity {g cm-3, for cluster ions typically 2.08}, ParticleCharge {e, for cluster ions 1}, MassDiameter {nm} : real) : real;
var p, q : real;
begin
  if x > 1 then Omegall := 1 + 0.106 / x + 0.263 / exp ((4/3) * ln (x))
  else begin p := sqrt (x); q := sqrt (p);
  Omegall := 1.4691 / p - 0.341 / q + 0.181 * x * q + 0.059 end;
end;
const GasMass = 28.96; {amu} Polarizability = 0.00171; {nm3}
a = 1.165; b = 0.48; c = 1.001; {the slip factor coefficients}
ExtraDistance = 0.115 {nm}; TransitionDiameter = 2.48 {nm};
var Temperature, GasDiameter, Viscosity, FreePath, DipoleEffect, DeltaTemperature, CheckMark, ParticleMass, CollisionDistance, Kn, Omega, s, x, y, r1, r2 : real;
```

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The reference model

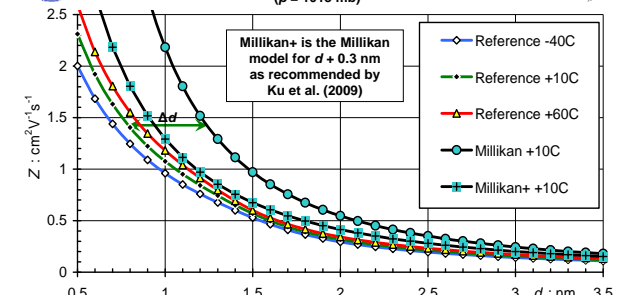
```
begin
  if MassDiameter < 0.2 then {emergency exit}
  begin electrical_mobility_air := 1e99; exit; end;
  Temperature := Celsius + 273.15;
  r1 := Temperature / 296.15; r2 := 406.55 / (Temperature + 110.4);
  Viscosity {microPa s} := 18.3245 * r1 * sqrt (r1) * r2;
  FreePath {nm} := 67.3 * sqrt (r1) * (1013 / millibar) * r2;
  ParticleMass {amu} := 315.3 * ParticleDensity * exp (3 * ln (MassDiameter));
  DeltaTemperature := Temperature;
  repeat
    CheckMark := DeltaTemperature;
    GasDiameter {nm} := 0.3036 * (1 + exp (0.8 * ln (44 / DeltaTemperature)));
    CollisionDistance {nm} := MassDiameter / 2 + ExtraDistance + GasDiameter / 2;
    DipoleEffect := 8355 * sqrt (ParticleCharge) * Polarizability / sqrt (sqrt (CollisionDistance));
    DeltaTemperature := Temperature + DipoleEffect;
  until abs (CheckMark - DeltaTemperature) < 0.01;
  if ParticleCharge = 0 then Omega := 1
  else Omega := Omegall (Temperature / DipoleEffect);
  Kn := FreePath / CollisionDistance;
  if Kn < 0.03 {underflow safe} then y := 0 else y := exp (- c / Kn);
  x := (273.15 / DeltaTemperature) * exp (3 * ln (TransitionDiameter / MassDiameter));
  if x > 30 {overflow safe} then s := 1
  else if x > 0.001
  then s := 1 + exp (x) * sqrt (x / (exp (x) - 1)) * (2.25 / (a + b) - 1)
  else {underflow safe} s := 1 + (2.25 / (a + b) - 1);
  electrical_mobility_air := 1.6022 * ((2.25 / (a + b)) / (Omega * s - 1)) * sqrt (1 + GasMass / ParticleMass) * (1 + Kn * (a + b * y)) / (6 * PI * Viscosity * CollisionDistance);
end;
```

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Experiment 1: $Z = f(d)$

($p = 1013$ mb)

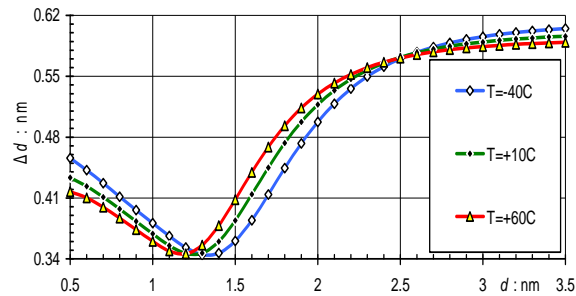


Studies of small ions and gas discharge estimate the mobilities of small molecular ions ($d \approx 0.4$ nm) at standard conditions about $2.2 \dots 2.5 \text{ cm}^2 \text{V}^{-1} \text{s}^{-1}$ and less. Millikan+ issues about $4 \text{ cm}^2 \text{V}^{-1} \text{s}^{-1}$.

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Experiment 2: Required Δd



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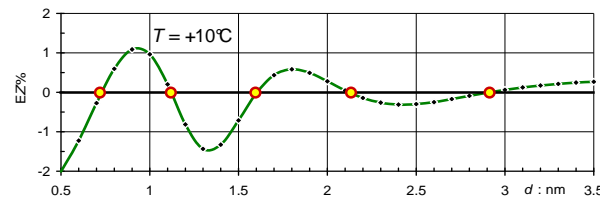
Experiment 3: Fitting of $\Delta d = f(d)$



$$Z_1 = f_{\text{MillikanZ}}(p, T, d + f_{\Delta 1}(d))$$

$$\Delta d \approx f_{\Delta 1}(d) = k_1 - k_2 \times \exp(-k_3 \times (d - k_4)^2) - k_5 / d$$

$$EZ = (Z_1 - Z_0) / Z_0$$



$$k_1 = 0.6 \quad k_2 = 0.22 \quad k_3 = 1.8 \quad k_4 = 1.2 \quad k_5 = 0.033$$

Five parameters, five zeros.

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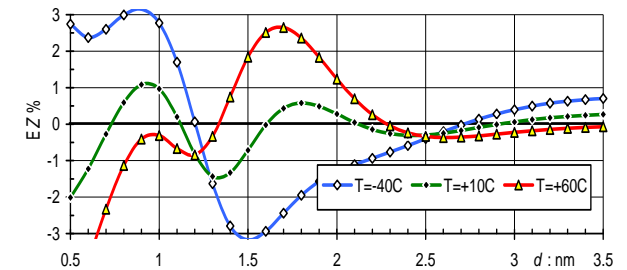
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$$Z_1 = f_{\text{MillikanZ}}(p, T, d + f_{\Delta 1}(d))$$

$$\Delta d \approx f_{\Delta 1}(d) = 0.6 - 0.22 \times \exp(-1.8 \times (d - 1.2)^2) - 0.033 / d$$

$$EZ = (Z_1 - Z_0) / Z_0$$



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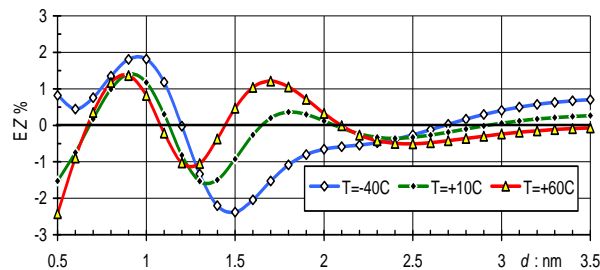


Experiment 4: Temperature correction



$$Z_2 = f_{\text{MillikanZ}}(p, T, d + f_{\Delta 2}(d, T))$$

$$f_{\Delta 2}(d, T) = 0.6 - 0.22 \times \exp(-1.8 \times (d + 0.001 \times T \times C - 1.2)^2) - 0.033 / d$$



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Accuracy of approximation $d = f(Z)$



Diameter is calculated by numerical inversion of the Millikan function.

The error of approximation = deviation of the diameter calculated according to the approximate model from the diameter calculated according to the reference model.

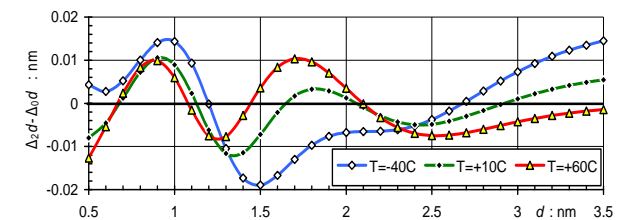
Estimating the error of approximation:

- choose a value of d_0 ,
- calculate $Z = f_{\text{reference}}(p, T, d_0)$,
- solve $Z = f_{\text{MillikanZ}}(p, T, d_2 + f_{\Delta 2}(d_2, T))$ for d_2 .
- absolute error = $d_2 - d_0$,
- relative error = $(d_2 - d_0) / d_0$.

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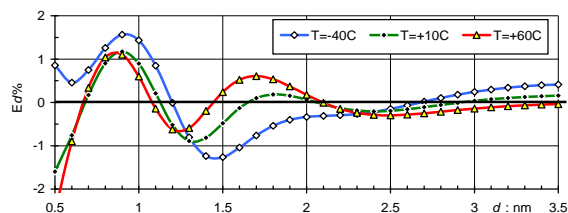
Experiment 5: absolute error of approximation $d = f(Z)$



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Experiment 6: relative error of approximation $d = f(Z)$



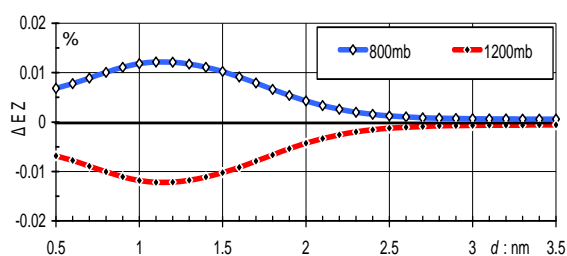
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Experiment 7: pressure error of $d = f(Z)$



$$\Delta EZ = EZ_p - EZ_{1000 \text{ mb}}$$



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The end of the discussion

Appendixes



Comparison of models



Program A_tools, see http://ael.physic.ut.ee/tammet/A_tools/

Electrical mobility (cm²V⁻¹s⁻¹) at 1013 mb and 10 °C:

d:nm	Millikan+	Tammet95	Reference	Approx	T95/Ref	Mkn+/Ref	Appr/Ref
0.6	2.48522	1.88764	1.92191	1.90759	0.9822	1.2931	0.9925
0.8	1.66449	1.38013	1.40518	1.41913	0.9822	1.1845	1.0099
1.0	1.19233	1.05643	1.07559	1.08827	0.9822	1.1085	1.0118
1.5	0.62271	0.55834	0.56846	0.56319	0.9822	1.0954	0.9907
2.0	0.38187	0.31324	0.31891	0.31930	0.9822	1.1974	1.0012
3.0	0.18597	0.15451	0.15730	0.15739	0.9823	1.1823	1.0006
5.0	0.07246	0.06379	0.06494	0.06511	0.9823	1.1159	1.0026
7.0	0.03839	0.03481	0.03543	0.03549	0.9824	1.0835	1.0017
10.0	0.01943	0.01804	0.01836	0.01838	0.9825	1.0587	1.0010
20.0	0.00514	0.00491	0.00499	0.00499	0.9830	1.0291	1.0003
50.0	0.00091	0.00088	0.00090	0.00090	0.9843	1.0112	1.0001

T95 is Tammet (1995) without corrections.
Mkn+ is updated Millikan for d+0.3 nm.

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Pascal



```
function Z_approx_air (millibar, Celsius, d [nm] : real) : real;
{cm2 V-1 s-1, mathematical approximation of mobility Tammet95m}
const a = 1.165; b = 0.48; c = 1.001; {Jung et al., 2011}
var Viscosity, FreePath, Kn, r1, r2, y, dd : real;
begin
  y := d + 0.001 * Celsius - 1.2;
  dd := d + 0.6 - 0.22 * exp (-1.8 * y * y) - 0.033 / d;
  r1 := (Celsius + 273.15) / 296.15;
  r2 := 406.55 / (Celsius + 383.55);
  Viscosity [microPa s] := 18.3245 * r1 * sqrt(r1) * r2;
  FreePath [nm] := 67.3 * sqrt(r1) * (1013 / millibar) * r2;
  Kn := 2 * FreePath / dd;
  if Kn < 0.03 {underflow safe} then y := 0 else y := exp (- c / Kn);
  Z_approx_air :=
    1.6022 * (1 + Kn * (a + b * y)) / (3 * PI * Viscosity * dd);
end;
```

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Excel



```
Sub Z_approx_air() ' HT 20120118
n = ActiveCell.Value
For i = 0 To n - 1
  mb = ActiveCell.Offset(i, -3).Value
  Celsius = ActiveCell.Offset(i, -2).Value
  d = ActiveCell.Offset(i, -1).Value
  y = d + 0.001 * Celsius - 1.2
  dd = d + 0.6 - 0.22 * Exp(-1.8 * y * y) - 0.033 / d
  r1 = (Celsius + 273.15) / 296.15
  r2 = 406.55 / (Celsius + 383.55)
  vi = 18.3245 * r1 * Sqr(r1) * r2
  fp = 67.3 * r1 * r1 * (1013 / mb) * r2
  Kn = 2 * fp / dd
  y = 0
  If Kn > 0.03 Then y = Exp(-1.001 / Kn)
  Z = 1.6022 * (1 + Kn * (1.165 + 0.48 * y)) / (3 * 3.14159 * vi * dd)
  ActiveCell.Offset(i, 0) = Z
Next i
End Sub
```

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Excel, inverse function



```
Sub d_approx_air() ' HT 20120118
n = ActiveCell.Value
For i = 0 To n - 1
  mb = ActiveCell.Offset(i, -3).Value
  Celsius = ActiveCell.Offset(i, -2).Value
  Z = ActiveCell.Offset(i, -1).Value
  r1 = (Celsius + 273.15) / 296.15
  r2 = 406.55 / (Celsius + 383.55)
  vi = 18.3245 * r1 * Sqr(r1) * r2
  fp = 67.3 * r1 * r1 * (1013 / mb) * r2
  c = 100
  m = 0
  OK = False
  While Not OK
    m = m + 1
    d = (0.6 + Sqr(0.36 + 200 * c * Z)) / (c * Z) - 0.4
    y = d + 0.001 * Celsius - 1.2
    dd = d + 0.6 - 0.22 * Exp(-1.8 * y * y) - 0.033 / d
    Kn = 2 * fp / dd
    y = 0
    If Kn > 0.03 Then y = Exp(-1.001 / Kn)
    test = 1.6022 * (1 + Kn * (1.165 + 0.48 * y)) / (3 * 3.14159 * vi * dd)
    c = (1.2 / (d + 0.4) + 200 / ((d + 0.4) * (d + 0.4))) / test
    OK = (Abs(test / Z - 1) < 0.000001) Or (m = 99)
  Wend
  If m > 99 Then d = 0
  ActiveCell.Offset(i, 0) = d
Next i
End Sub
```

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Excel, how to use?



- Text of both macros is available in the document http://ael.physic.ut.ee/tammet/A_tools/Size-mobility-approx.pdf. Select and copy the text of one or two macros to the clipboard.
- Open an Excel worksheet. Choose tools → macro → record new macro → store macro in this workbook → OK. A tiny recorder toolbar will appear. Remember the macro name and press the lower left button. The toolbar disappears and a new empty macro is saved.
- Choose tools → macro → macros → name of the new empty macro → edit. VBA window will appear. Select full text of the empty macro and paste the text from the clipboard as a replacement.
- Go back to the Excel worksheet, fill three neighbor columns in the worksheet with values of air pressure (mb), temperature (Celsius), and mobility (cm²V⁻¹s⁻¹), write number of rows to be processed into the cell just right of the first value of the mobility (see the example) and click this cell. NB: all data must be presented as values.
- Choose tools → macro → macros → name of macro → RUN.

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Excel, how to use?



p:mb	T:°C	Z:cm ² V ⁻¹ s ⁻¹	d:nm
1013	0	0.5	4
1013	10	0.5	
990	20	1	
990	20	2	

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Excel, how to use?



p:mb	T:°C	Z:cm ² V ⁻¹ s ⁻¹	d:nm
1013	0	0.5	1.5816
1013	10	0.5	1.5940
990	20	1	1.0959
990	20	2	0.5986

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